

2-METHYLHEXANEDIOIC ACID
33659-32-4 | DTXSID20334839

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 1.37e-01 mol/L

Global applicability domain: Inside

Local applicability domain index: 6.98e-01

Confidence level: 5.79e-01

Nearest Neighbors from the Training Set

Image not found

Heptanedioic acid

Measured: 3.12e-01

Predicted: 1.47e-01

Image not found

Propionic acid, 3,3'-diselenodi-

Measured: 5.39e-03

Predicted: 1.65e-02

Image not found

Octanedioic acid

Measured: 6.79e-02

Predicted: 4.83e-02